Module 1: Evaluating Environmental Partitioning and Fate: Approaches based on chemical structure

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Module 1: Evaluating Environmental Partitioning and Fate: Approaches based on chemical structure

- Educational goals and topics covered in the module
- Potential uses of the module in chemical engineering courses
- Student handouts
- Instructor materials and textbook
- Software
- Case studies

Module 1: Educational goals and topics covered in the module

Students will:

- become aware of the chemical and physical properties that govern a chemical's environmental partitioning and fate
- be able to estimate properties that govern environmental partitioning and fate based on chemical structure
- be able to perform mass balances to estimate environmental partitioning and be able to design structures that have targeted properties
- be aware of the limitations of structure-property estimation methods

Module 1: Educational goals and topics covered in the module (cont'd)

Properties covered:

- Properties used to estimate partitioning:
  boiling point, vapor pressure, octanol-water partition coefficient, bioconcentration factor, Henry's law coefficient, soil sorption
- Properties that govern environmental fate:
  atmospheric lifetimes, biodegradation rates
- Typical values of properties
- Environmental partitioning calculations

Module 1: Potential uses of the module in chemical engineering courses

- Design course: Use as a preliminary screen of chemical products and raw materials, prerequisite for module 2 (TSCA PMN)
- Materials course/thermodynamics course: Module on estimating properties
- Mass and energy balances course: module on estimating mass partitioning in closed systems

Module 1: Student handouts

- Chapter 5 from textbook: ***Evaluating Environmental Partitioning and Fate : Approaches based on chemical structure***
- Class lecture notes: edited from chapter 5 and designed so that instructor writes in key concepts and calculations during the lecture
- Problem 1: Environmental partitioning and fate
- Problem 2: Design of a solvent

Module 1: Instructor materials

- Completed class lecture notes: edited from chapter 5; contains material that the instructor writes into the notes during the lecture
- Problem 1: Environmental partitioning and fate: solution
- Problem 2: Design of a solvent: solution
- Software for estimating properties

Module 1: Software

EPIWIN collection of software programs - Properties covered:

- Properties used to estimate partitioning: boiling point, vapor pressure, octanol-water partition coefficient, bioconcentration factor, Henry's law coefficient, soil sorption
- Properties that govern environmental fate: atmospheric lifetimes, biodegradation rates

EPIWIN:
Software Demonstration

Module 1, Case study 1: Environmental partitioning case study

During pesticide application, 1 kg of hexachlorobenzene is accidentally applied to a 10^8 liter pond. Estimate the amount of hexachlorobenzene that would be ingested if a person were to eat a 0.5 kg fish from the pond. Assume that the pond is well mixed and that the organic sediment content is 10 ppm and the total fish loading is 100 g per 100 cubic meter.

Case study 1

- Decide what properties need to be calculated (Bioconcentration factor, octanol-water partition coefficient, soil/sediment sorption coefficient, Henry's law coefficient)
- Ratio all concentrations to the concentration in water
- Perform a mass balance
- Determine exposure

Solution

- Decide what properties need to be calculated

  octanol-water partition coefficient = $10^{5.9}$

  Bioconcentration factor = 6500

  soil/sediment sorption coefficient = 790 $\frac{\text{microgram/g. org C}}{\text{microgram/ml}}$

- Ratio all concentrations to the concentration in water
- Perform a mass balance

$$10^3 \text{ g} = 10^8 \text{ L}*(10^3 \text{ g/L})*C_w$$
$$+ 10^{11} \text{ g water} * 1 \text{ g sediment}/10^5 \text{ g water} * C_w * 790$$
$$+ 10^{11} \text{ g water} * 100 \text{ g biota}/10^8 \text{ g water} * C_w * 6500$$
$$C_w = 10 \text{ ppb}$$

- Determine exposure (6500 * 10 ppb) gives 6.5 * 10^{-5} g/g fish

  A 500 g fish results in ingestion of 0.0325 g

Module 1, Case study 2:

Design of a solvent molecule

- Motivation
- Edisonian approaches to solvent identification
- Group contribution methods
- Designing solvent molecules